Macromolecules

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Supplementary tables

Table S-I. Fractional coordinates of the Lovinger structure III_{au} obtained by optimization, using MSXX. The cell is orthorhombic with a= 9.68 Å, b= 4.98 Å, and c=9.13 Å. The space group is $Pca2_1(C_{2v}^5)$.

Atom	X	Y	Z
C_1	0.248	0.730	0.917
C_2	0.370	0.818	0.825
C_3	0.368	0.718	0.667
C_4	0.242	0.802	0.579
F_1	0.491	0.732	0.886
F_2	0.382	0.090	0.827
F_3	0.128	0.681	0.637
F_4	0.218	0.069	0.596
H_1	0.155	0.824	0.877
H_2	0.236	0.515	0.908
H_3	0.461	0.796	0.616
H_4	0.375	0.502	0.666

Table S-II. Piezoelectric constants g_{iJ} (C/m^2) calculated at the experimental structures (except for form III_{au}, where the optimized structure is used).

MSXX						MSXXS					
Form I_p											
0.0	0.0	0.0	0.0	-0.15	0.0	0.0	0.0	0.0	0.0	-0.15	0.0
0.0	0.0	0.0	-0.024	0.0	0.0	0.0	0.0	0.0	-0.067	0.0	0.0
-0.007	-0.01	-0.15	0.0	0.0	0.0	0.087	-0.073	-0.22	0.0	0.0	0.0
Form III_{pu}											
0.057	0.059	-0.19	0.0	-0.004	0.0	0.12	0.062	-0.26	0.0	-0.006	0.0
0.0	0.0	0.0	0.007	0.0	0.048	0.0	0.0	0.0	0.031	0.0	0.034
0.017	-0.017	0.18	0.0	0.071	0.0	0.032	0.0036	0.19	0.0	0.074	0.0
Form II_{pd}											
0.0	0.0	0.0	0.0	0.067	0.0	0.0	0.0	0.0	0.0	0.069	0.0
0.0	0.0	0.0	0.045	0.0	0.0	0.0	0.0	0.0	0.032	0.0	0.0
-0.21	0.030	0.023	0.0	0.0	0.0	-0.27	0.028	0.089	0.0	0.0	0.0
Form III_{au}											
0.0	0.0	0.0	0.0	-0.0002	0.0	0.0	0.0	0.0	0.0	0.024	0.0
0.0	0.0	0.0	0.0096	0.0	0.0	0.0	0.0	0.0	0.012	0.0	0.0
-0.026	0.024	0.18	0.0	0.0	0.0	-0.011	0.042	0.18	0.0	0.0	0.0

Table S-III. Elastic constants(C_{IJ} in GPa) and piezoelectric moduli (d_{iJ} in pC/N) of PVDF form I_p.

	TKTF[a]	MSXXS	MSXX	Exper
C_{11}	23.60	23.7	25.5	
C_{22}	10.64	11.8	12.4	
C_{33}	238.24	266.8	283.4	
C_{12}	1.92	2.4	3.0	
C_{13}	3.98	4.7	4.0	
C_{23}	2.19	3.1	2.4	
C_{44}	4.40	3.7	3.5	
C_{55}	6.43	5.2	5.1	
C_{66}	2.15	4.0	4.0	
d_{15}	-30.70	-41.9	-41.3	
d_{24}	-4.28	-16.8	-5.9	-38.3[c]
d_{31}	-0.25	0.57	0.07	
d_{32}	-4.05	-1.3	1.1	
d_{33}	-25.19	-18.8	-12.7	-20 ± 5[b]

[a] Reference 23.

[b] Reference 23.

[c] Reference 26.